

N89-21748

1988

NASA/ASEE SUMMER FACULTY FELLOWSHIP PROGRAM

MARSHALL SPACE FLIGHT CENTER
THE UNIVERSITY OF ALABAMA

ELECTRON MOBILITY IN MERCURY CADMIUM TELLURIDE

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Date:	August 19, 1988
Contract No.:	NGT 01-002-099 The University of Alabama

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ABSTRACT

A previously developed program, which includes all electronic interactions thought to be important, does not correctly predict the value of electron mobility in mercury cadmium telluride particularly near room temperature. Part of the reason for this discrepancy is thought to be the way screening is handled. It seems likely that there are a number of contributors to errors in the calculation. The objective of this work is to survey the calculation, locate reasons for differences between experiment and calculation, and suggest improvements.

ACKNOWLEDGMENTS

The author wishes to thank the NASA/ASEE Summer Faculty Fellowship Program. Special thanks are due Dr. Mike Freeman, UA University Programs Co-Director and Ernestine Cothran, NASA MSFC Program Director.

Thanks are especially expressed to NASA Colleague Sandor L. Lehoczky and to Frank Szofran of the Space Science Laboratory.

The author is grateful to Shirley A. Buford, of the Crystal Growth Branch, for typing this manuscript.

Finally the author is grateful to the Administration of the Florida Institute of Technology for granting a leave of absence which allowed participation in this program.

1. Introduction

Many relevant properties of and references about $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ have already been given (Patterson (1987), see also Appendix 1).

The calculation of the transport properties of narrow band gap semiconductors (of which mercury cadmium telluride is an important example) have met with considerable success (Lehoczky et al. (1982), Szymanska et al. (1978), and Chattopadhyay and Nag (1974)). Nevertheless it is not unusual to find calculations (near room temperature) differing from experiment by a factor of order two.

The original idea of this project was that inadequate treatment of screening was the cause of discrepancies between calculation and experiment. However, in a calculation as complex as the mobility of electrons in a narrow band gap semiconductor (see Appendices 2 and 3) even the accuracy of the present calculations would have to be regarded as good (Lehoczky et al. (1980)).

An easy way to test the importance of screening is to run the present codes with different values of the screening constants. As we will see such calculations lead one to feel there is a limit to the accuracy with which the mobility can be evaluated, and certainly a limit to how much the accuracy can be improved by improving the screening.

2. Objectives

a. Determine the effect on the mobility of electrons in $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ of variations in relevant parameters. Pay particular attention to screening parameters.

b. Survey the theory on which the calculation is based to try to pinpoint areas that can be improved.

3. Calculations

We start by observing that in the approximation considered, the effects of screening are determined by the screening lengths. There exist reasons for considering other values of these lengths beside the conventional one (Patterson, (1987), appendices 3 and 5). Thus we are motivated to consider the results of calculations in which the screening length is varied for fixed values of the other parameters.

We also show how variations in screening affect the results for different values of the Cd concentration (x). All our results are based on a program of Dr. S.L. Lehoczky as rewritten by Ernestine Cothran. The program considers electron interaction effects due to longitudinal optic phonons, ionized impurities, holes, acoustic phonons, compositional disorder and neutral defects.

In what follows, we present our calculations in terms of hypotheses and calculational tests of the hypotheses.

Hypothesis

Although screening is important sizable changes in screening are not sufficient to get agreement with experiment.

TEST (μ is the mobility, k_{TF} represents all Fermi-Thomas wave vectors and T is the temperature).

$$f_E \equiv \frac{\mu(.5 k_{TF}^2, \chi=.183) - \mu_{exp}}{\mu(k_{TF}^2, \chi=.183) - \mu_{exp}},$$

at T = 300K, $n_D = 5.6 \times 10^{14} \text{ cm}^{-3}$ (the donor concentration)

$$f_E \approx .742,$$

at T = 100K, $n_D = 5.6 \times 10^{14} \text{ cm}^{-3}$

$$f_E \approx .665.$$

This is further shown by Figs. 1a and 1b where one sees that it is necessary (for the example shown) to use .05 of the nominal values for k_{TF}^2 in order to obtain near agreement with experiment.

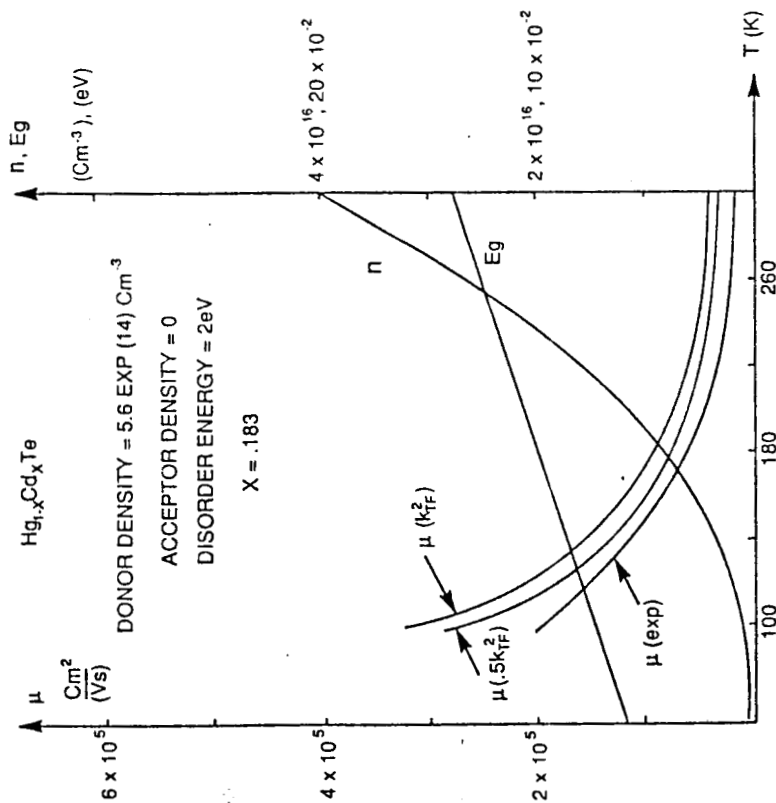


FIG. 1A

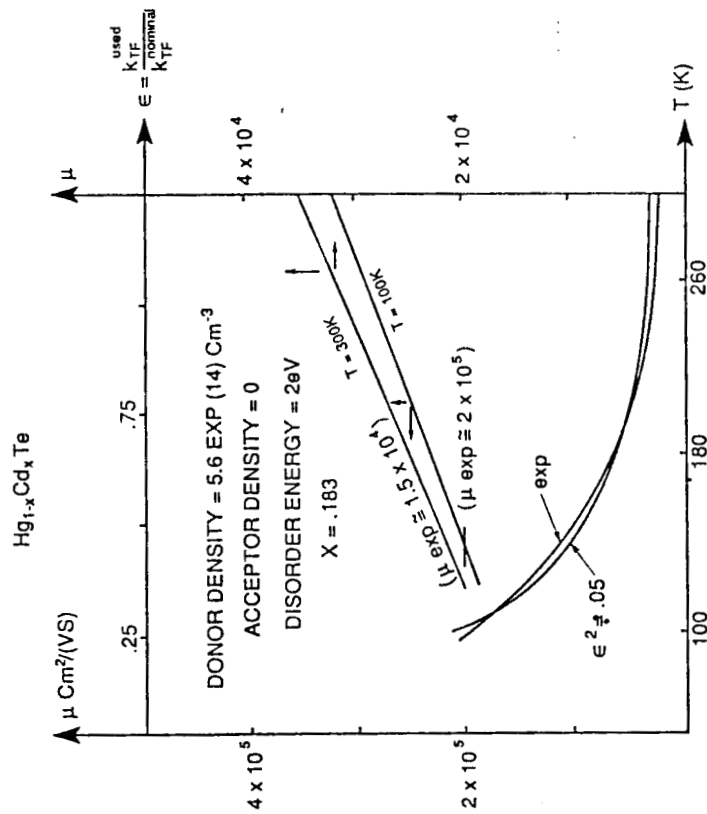


FIG. 1B

FIG. 1 (A) ELECTRON MOBILITY μ (cm^2/Vs) VS TEMPERATURE T (K), ALSO ENERGY GAP E_g AND ELECTRON CONCENTRATION N VS TEMPERATURE; (B) ELECTRON MOBILITY VS T AND SCREENING STRENGTH $\epsilon = k_{IF}^{\text{used}} / k_{IF}^{\text{nominal}}$.

Hypothesis

The mobility varies monotonically (very roughly linearly) as a function of inverse screening length (k_{TF}).

$$\epsilon^2 \equiv k_{TF}^{2 \text{ (used)}} / k_{TF}^{2 \text{ (nominal)}}$$

Test

at $x = .183$, $T = 100K$, $n_D = 5.6 \times 10^{14} \text{ cm}^{-3}$ ($\mu_{\text{exp}} \approx 200 \times 10^3 \frac{\text{cm}^2}{\text{Vs}}$)

ϵ^2	ϵ	μ	$\Delta\mu / \Delta\epsilon$
1	1	322,205	141,582
.75	.866	303,233	138,157
.5	.707	281,266	138,469
.25	.5	252,603	142,453
.2	.447	245,053	150,344
.1	.316	225,358	169,076
.05	.224	209,803	212,629
.01	.1	183,437	

at $x = .183$, $T = 300K$, $n_D = 5.6 \times 10^{14} \text{ cm}^{-3}$ ($\mu_{\text{exp}} \approx 15 \times 10^3 \frac{\text{cm}^2}{\text{Vs}}$)

ϵ^2	ϵ	μ	$\Delta\mu / \Delta\epsilon$
1	1	35,160	18,529
.75	.866	32,677	17,113
.5	.707	29,956	16,184
.25	.5	26,606	15,641
.2	.447	25,777	15,908
.1	.316	23,693	16,902
.05	.224	22,138	20,452
.01	.1	19,602	

Hypothesis

The more carriers, the more screening we should have. Thus, the more the calculation should depend on variations in the screening length. Three ways the number of carriers can be varied are by varying the Hg concentration, varying the temperature T or varying the donor concentration.

Tests (These imply the above hypothesis is naive.)

at $T = 300K$, $\eta_D = 5.6 \times 10^{14} \text{ cm}^{-3}$

$$S_x = \frac{\mu(k_{TF}^2, x=.183) - \mu(.5k_{TF}^2, x=.183)}{\mu(k_{TF}^2, x=1) - \mu(.5k_{TF}^2, x=1)} = 5.004$$

at $x = .183$, $\eta_D = 5.6 \times 10^{14} \text{ cm}^{-3}$

$$S_T = \frac{\mu(k_{TF}^2, T=300) - \mu(.5k_{TF}^2, T=300)}{\mu(k_{TF}^2, T=100) - \mu(.5k_{TF}^2, T=100)} = .127$$

at $x = .183$ $T=300K$ $\eta_D = 5.6 \times 10^{14} \text{ cm}^{-3}$

$$S_{\eta_D} = \frac{\mu(k_{TF}^2, 2\eta_D) - \mu(.5k_{TF}^2, 2\eta_D)}{\mu(k_{TF}^2, \eta_D) - \mu(.5k_{TF}^2, \eta_D)} = 1.004$$

Hypothesis

At a fixed temperature, changes due to screening are more important for smaller band gaps. This is shown clearly in the Figs. 2a and 2b.

A simple expression for the energy gap as a function of temperature and x is given by Dornhaus and Nimtz (1983) who also list more accurate expressions. The expression is only supposed to be used for $.135 \leq x \leq .203$. In the table below the energy gap is evaluated from a slightly better expression in the program.

$$E_g = -.3 + 5 \times 10^{-4} T + (1.91 - 10^{-3} T)x \text{ in eV.}$$

We find at $T = 300K$,

$$E_g = -.15 + 1.61x.$$

If x_0 is the value of x for which the energy gap vanishes, we find for $T = 100$ that $x_0 = .138$.

Define $f_s = \frac{\mu(.5 k_{TF}^2, x)}{\mu(k_{TF}^2, x)}$, $\Delta = \mu(k_{TF}^2, x) - \mu(.5 k_{TF}^2, x)$.

For $n_D = 5.6 \times 10^{14} \text{ cm}^{-3}$ and $T = 300K$

x	$E_g(\text{eV})$	$n_E (\text{cm}^{-3})$	$\mu(.5 k_{TF}^2)$	$\mu(k_{TF}^2)$	f_s	Δ	$\Delta/\mu(k_{TF}^2)$
.14	.085	7.85×10^{16}	41,971 cm^2/vs	54,805	.766	12,834	.234
.15	.098	6.79 "	39,160	49,705	.788	10,545	.212
.16	.110	5.82	36,247	44,930	.807	8,683	.193
.17	.123	4.94	33,425	40,407	.827	6,982	.173
.18	.136	4.15	30,732	36,312	.846	5,580	.154
.19	.149	3.47	28,212	32,620	.865	4,408	.135
.20	.162	2.88	25,884	29,370	.881	3,486	.119

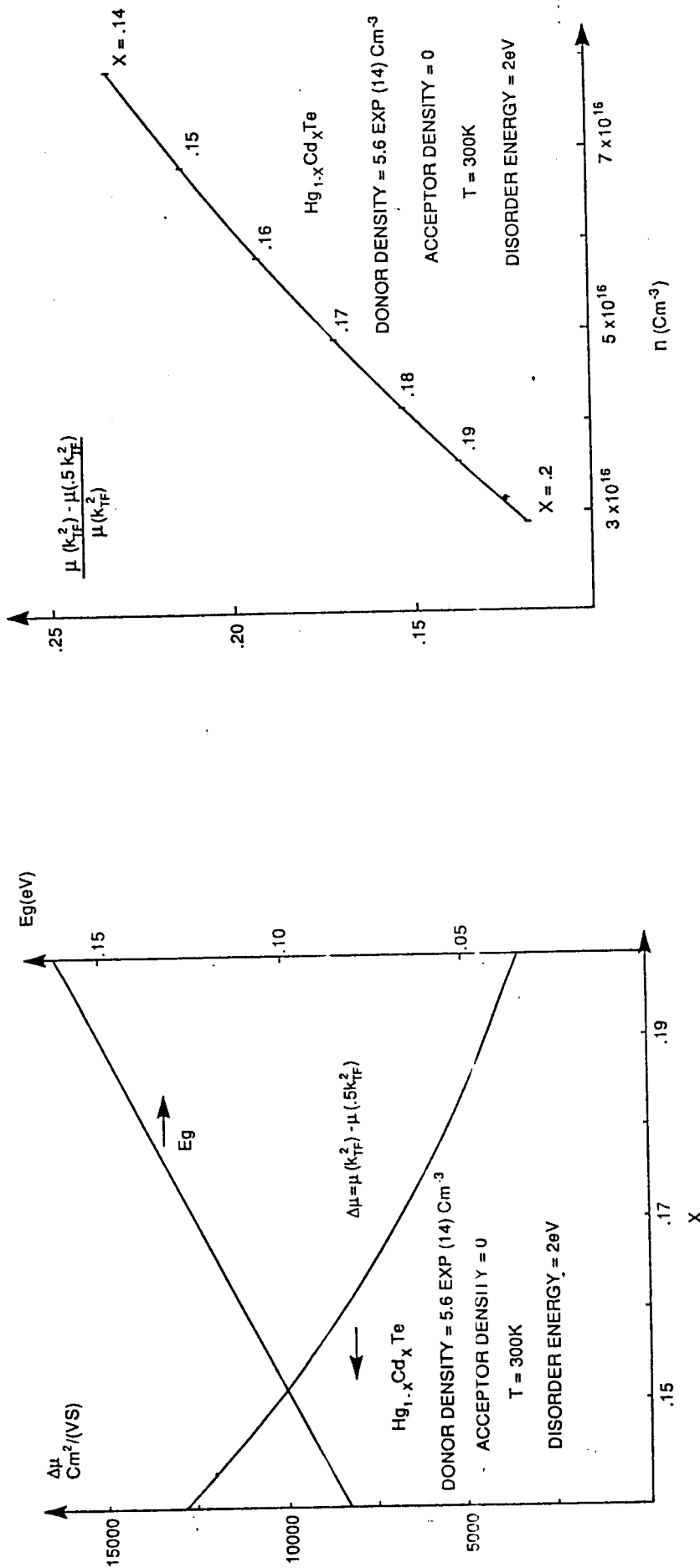


FIG. 2A

FIG. 2B

FIG 2. (A) ENERGY GAP E_g (eV) AND CHANGE IN MOBILITY $\Delta\mu$ (cm^2/Vs) ;
 (B) FRACTIONAL CHANGE IN MOBILITY VS ELECTRON CONCENTRATION.

4. Conclusions and Recommendations

a. Screening is important but it is not the whole answer. There are undoubtedly several small corrections.

b. In a calculation as complex as this one, see Figs. 3a and 3b and the appendices, the existing calculation (Lehoczky (1980), (1982)) is already good. See also Nag (1980) for comparison.

c. Small corrections and rewriting the code for a more modern computer are realistic goals for improvement. The program is presently implemented in basic for an HP 9845B and it runs rather slowly.

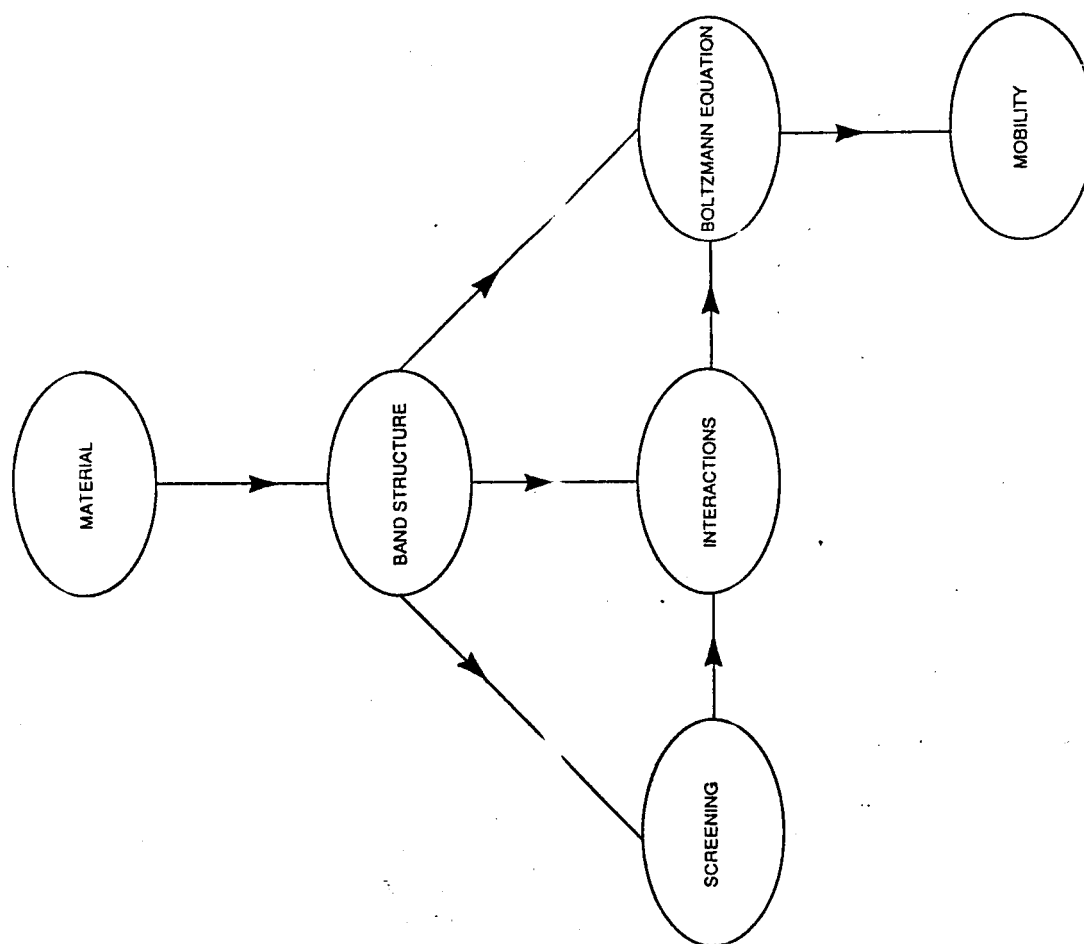


FIG. 3A

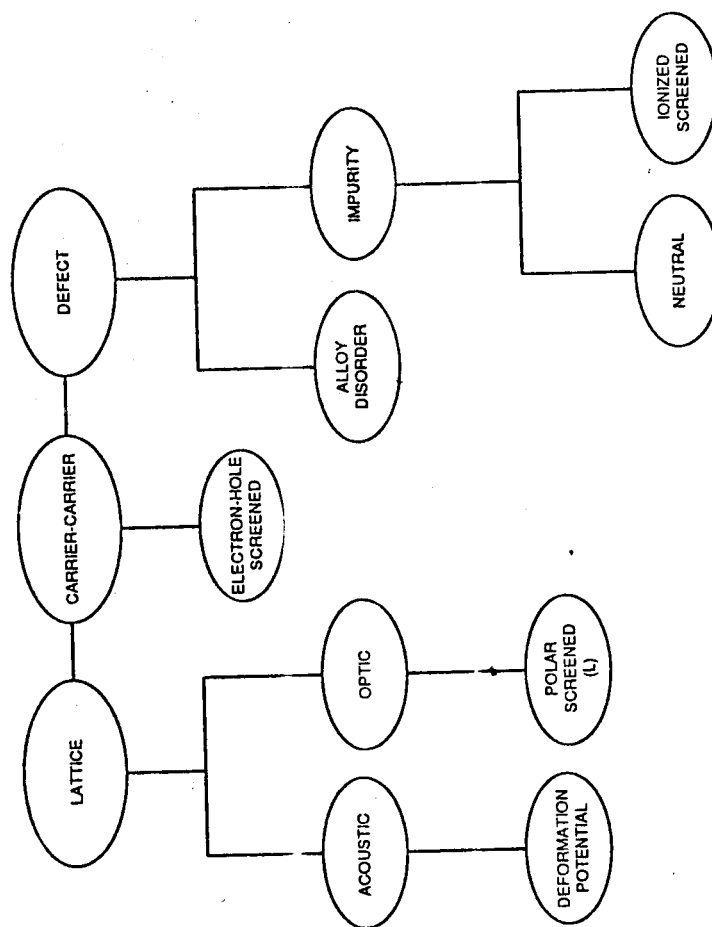


FIG. 3B

FIG. 3: THE CALCULATION; (A) OVERVIEW; (B) SCATTERING MECHANISMS.

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Appendix 1

Brief Properties of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$:

1. Pseudo Binary II-VI Compound with structure isomorphic to zincblende.
2. The bandgap is tunable from 0 to 1.605 eV as x goes from about .17 (at low temperature) to 1.0. The bandgap also depends on temperature. $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ forms a continuous range of solid solutions between the semimetal HgTe and the semiconductor CdTe.
3. Can use as an infrared detector at liquid nitrogen temperature in the wavelength range 8-12 μ - an atmospheric window. A higher operating temperature than alternative materials, high detectivity, fast response, high sensitivity, IC compatible and low power.
4. Candidate for microgravity crystal growth.
5. Band structure involves mixing of unperturbed valence and conduction band wave functions as derived by the Kane theory. Non parabolic bands.
6. Typical carriers have small effective mass (about 10^{-2} * free electron mass) which implies large mobility. The effective mass also has a strong dependence on concentration and temperature.
7. Polar scattering by LO lattice vibration modes dominate above 77K (or so) and the relaxation time approximation is not valid. The scattering is inelastic since the phonon energy is comparable to the electron energy.
8. Narrow bandgap semiconductors imply thermally excited electrons and hence screening. There may also be antiscreening effects when the phonons have higher phase velocity than the Fermi velocity of electrons.

Dornhaus and Nimtz (1983) list many more properties.

Appendix 2

Boltzmann Transport Equation and Solution

We just have a few comments to make here as the Boltzmann Transport equation is well reviewed in several texts (Blatt (1968), Wilson (1958)).

If f is the distribution function (with f_0 its value in equilibrium), E the energy, and if terms of order Φ^2 are neglected where

$$f = f_0 - \Phi(\vec{k}) \frac{\partial f_0}{\partial E}, \quad (A2.1)$$

then with electric fields \vec{E} and temperature (T) gradients in the x -direction

$$\begin{aligned} v_x \frac{\partial f_0}{\partial E} \left[|e| E_x + \frac{\partial E_F}{\partial x} + \left(\frac{E - E_F}{T} \right) \frac{\partial T}{\partial x} \right] \\ = \frac{1}{kT} \int V(\vec{k}, \vec{k}') [\Phi(\vec{k}) - \Phi(\vec{k}')] d\vec{k}', \end{aligned} \quad (A2.2)$$

where E_F is the Fermi energy v_x is the velocity, \vec{k} the wave vector, $|e|$ the magnitude of electronic charge, and $V(\vec{k}, \vec{k}')$ is determined by the electron scattering mechanism (it is proportional to the probability of scattering from \vec{k} to \vec{k}').

Since some of the scattering mechanisms are inelastic a variational principle is used to solve for $\Phi(\vec{k})$. The work is detailed, but well described ((Wilson (1958) Lehoczky (1980)). From f , the current density J_x (with $\frac{\partial T}{\partial x} = 0$) is

$$J_x = - \frac{|e|}{4\pi^3} \int f v_x d\vec{k}, \quad (A2.3)$$

and the mobility is $\mathcal{M} = J_x / (\eta |e| E_x)$, where η is the electron concentration.

Appendix 3

Electron Scattering Mechanisms

The details here are too long to write down. Fortunately they have already been well described (Lehoczky (1980), Lehoczky (1974), Nelson (1978), Dubowski (1981), Ehrenreich (1959), Zawadzki (1974), and Szymanska (1978)). Special mention should be made of Ehrenreich who wrote many of the key papers in this area. They are referenced in the above references.

a. Electron-phonon Interaction in Polar Solids

The only strong interactions are with longitudinal optic modes and we will limit discussion to long wave length modes near the center of the Brillouin zone with frequency ω_L . Several approximations then follow for which the literature may be consulted.

$$H_{el-ph} = \sum_{\vec{q}, \vec{k}, \sigma} \frac{M}{q \epsilon(\omega_L, q)} (a_{\vec{q}} + a_{-\vec{q}}^+) C_{\vec{k}+\vec{q}, \sigma}^+ C_{\vec{k}, \sigma} \quad (A3a.1)$$

The a's are the phonon annihilation and creation operators and the c's are the electron creation and annihilation operators. M is an appropriately chosen constant.

The screening is included by using the dielectric function

$$\epsilon(\omega_L, q) = \epsilon_{\infty} + \frac{(k_{FT}^e)^2 + (k_{FT}^{lh})^2}{q^2}, \quad (A3a.2)$$

and a "two mode" theory is necessary (with frequencies close to those of CdTe and HgTe). ϵ_{∞} is the high frequency dielectric constant.

Further Comment Screening and Antiscreening

Our main point here is to point out that antiscreening at small wave vectors can account for increased interaction and hence reduced scattering. This can occur when phonons with small wave vector also have high phase velocity which can occur for optical modes. As Ehrenreich (1959) has shown, the screened potential can actually be greater than the unscreened one.

b. Charged Impurity and the Friedel Sum Rule

This is also referred to as ionized impurity scattering (ii):

$$H_{ii} = \sum_{\vec{k}, \vec{q}} \sum_{\sigma} F_{\vec{k}+\vec{q}, \vec{k}} \frac{V(q)}{\xi(q)} C_{\vec{k}+\vec{q}, \sigma}^{\dagger} C_{\vec{k}, \sigma}, \quad (A3b.1)$$

where

$$F_{\vec{k}+\vec{q}, \vec{k}} = \frac{1}{\Omega} \int u_{\vec{k}+\vec{q}}^{\star}(\vec{r}) u_{\vec{k}}(\vec{r}) dV, \quad (A3b.2)$$

with $u_{\vec{k}}(\vec{r})$ being the periodic modulation of the plane wave in Bloch's theorem and is often not included. $V(q)$ is the Fourier transform of the Coulomb potential. Screening is included by $\xi(q)$ and

$$\xi(q) = \xi_0 + \frac{1}{q} \left[(k_{FT}^e)^2 + (k_{FT}^{lh})^2 + (k_{FT}^{hh})^2 \right], \quad (A3b.3)$$

where ξ_0 is the low frequency dielectric constant.

Screening was more fully discussed in the first report (Patterson, 1987). Briefly, if a charge is placed in an electron gas its potential is better described by $e^{-\lambda r}/r$ than $1/r$ because the electrons in the gas surround the charge and "screen" it. The screening length is defined as λ^{-1} . The process is best described by a wave vector dependent dielectric constant, as above.

Further Comments: Multiple Scattering and Other Corrections to Calculations

Chattopadhyay and Queisser (1981) have discussed corrections due to multiple scattering and impurity dressing. The usual assumption with regard to ionized impurity scattering is that each impurity scatters independently. Multiple scattering adds corrections due to the electron interacting with more than one ion simultaneously. There is also a correction due to the fact that the impurities perturb the electron energies and wave functions. This is called the dressing correction and it can amount to 50% or so of the multiple scattering correction. However the corrections to ionized impurity scattering are not very important compared to other scattering mechanisms in $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ at temperatures of interest here. The dressing and multiple scattering corrections to ionized impurity scattering are more important at higher temperatures and lower impurity concentrations.

Corrections to the Born approximation (in a calculation of ionized impurity scattering) can also be important at lower temperature but second order Born corrections are probably only useful if they are small.

An expression for the screening length $L = \lambda^{-1}$ is given in appendix 5. It is possible to derive this directly or by use of the first Born approximation and the Friedel sum rule involving phase shifts δ_l (see e.g. Joachain, 1975). The Friedel sum rule holds generally and is supposed to be exact. It holds even for interacting electrons in a periodic system. The essential physical contents of the Friedel sum rule is the requirement of overall electrical neutrality about the charged ion. For electrons in a semiconductor, the Friedel sum rule takes the form, in the usual notation;

$$Z = (2/\pi) \sum_l (2l+1) \int \frac{d\delta_l}{dE} f(E) dE. \quad (A36.4)$$

c. Electron-Hole

When the heavy hole mass is large compared to the electron mass the hole can be considered to be stationary during scattering. This would make electron-hole scattering theory formally identical to ionized impurity scattering.

However we still must include non parabolity and admixture of p wave functions into the conduction band. For details see the references.

This is also a screened interaction. The following dielectric function has been used

$$\epsilon(q) = \epsilon_{\infty} + \frac{(k_{FT}^e)^2 + (k_{FT}^{eh})^2 + (k_{FT}^{hh})^2}{q^2} \quad (A3C.1)$$

d. Electron-Acoustic phonon

For semiconductors this is often treated by using the idea of a deformation potential (Seeger 1985, Madelung, 1978). If E_0 is the bottom of the conduction band then if E is the energy of the electron, we can obviously write

$$E = (E - E_0) + E_0, \quad (A3d.1)$$

where $(E - E_0)$ is treated as the kinetic energy and E_0 is viewed as the potential energy. One can think of E_0 varying with long wavelength displacements (\vec{J}) and this variation produces the deformation potential and thus the electron lattice coupling. At long wavelengths, Umklapp processes can be neglected. We write

$$H_{el-ph} = \frac{\partial E_0}{\partial V} \Delta V = \frac{\partial E_0}{\partial V} V \vec{\nabla} \cdot \vec{J} \propto \vec{J} \cdot \vec{g}, \quad (A3d.2)$$

for a single wave with wave vector \vec{g} . Further generalization leads to putting this in the usual form (see references). In the above V is the volume.

In the actual calculations, both longitudinal (L) and transverse (T) scattering is included by the use of three deformation potentials (1L, 2T).

e. Compositional Disorder and Neutral Defect
Compositional Disorder

This is calculated by considering a random distribution of scattering centers consisting of square wells.

The square wells are chosen to have a size equivalent to a unit cell and a depth (E_d) determined by the differences in band gaps between CdTe and HgTe.

If N_a is the number of unit cells per unit volume

$$\left. \frac{\partial f}{\partial t} \right)_{\text{dis. scatt}} \propto \frac{x(1-x) E_d^2}{N_d}, \quad (\text{A3c.1})$$

(see Lehoczky et al., (1980)).

The dependence on $x(1-x)$ is known as Nordheim's rule. For a given x , $x(1-x)$ measures the disorder assumed to be present (maximum).

Neutral Defect Scattering

This is also described as scattering by a random distribution of square-well potentials. It has been neglected in this calculation, but one assumes

$$\left. \frac{\partial f}{\partial t} \right)_{nd} \propto x(1-x) N E^2 V^2, \quad (\text{A3c.2})$$

(see Lehoczky et al., (1980)),

where N is the density of neutral defects, E is their strength and V is the volume of the cell.

Appendix 4

The Polaron Constant

The Polaron constant α is defined, in the usual notation, as

$$\alpha = \frac{e^2}{\hbar} \sqrt{\frac{m^*}{2\hbar\omega_L}} \left(\frac{1}{\epsilon(\infty)} - \frac{1}{\epsilon(0)} \right), \quad (A4.1)$$

It is a measure of the strength of the electron-lattice interaction and is dimensionless. For the phonon field and electrons to interact weakly we need $\alpha < 1$. For the Frohlich interaction term to be valid we also need $\alpha < 1$.

To get an estimate of α we use the following values:

$$\begin{aligned} \epsilon(\infty) &= 15, & |e| &= 4.8 \times 10^{-10} \text{ esu} \\ \epsilon(0) &= 20, & \hbar &= 1.05 \times 10^{-27} \text{ erg-s} \\ m^* &= .03m, & m &= 9.1 \times 10^{-28} \text{ gm} \\ \hbar\omega_T &= 2.4 \times 10^{-14} \text{ ergs} \end{aligned}$$

Thus

$$\alpha \cong .092.$$

Appendix 5

Band Structure and Effective Masses

We briefly summarize Kane (1957) theory here. We give some idea of the band structure near the top of the valence band and bottom of the conduction band. A simple schematic diagram of the band structure has been given by Seeger (1985), see also Lehoczky (1974). The s wave functions of the conduction band are found to mix with the p wave functions of the valence band by $\vec{k} \cdot \vec{p}$ perturbation theory (for $\vec{k} \neq 0$).

By using Bloch's theorem the wave function is given by

$$\psi_{n\vec{k}}(\vec{r}) = u_{n\vec{k}}(\vec{r}) e^{i\vec{k} \cdot \vec{r}}, \quad (A5.1)$$

in the usual notation. The Schrodinger wave equation can be written:

$$(H_0 + H') u_{n\vec{k}}(\vec{r}) = E_n' u_{n\vec{k}}(\vec{r}), \quad (A5.2)$$

where

$$H_0 = \frac{p^2}{2m} + V(\vec{r}) \quad (A5.3)$$

$$H' = \frac{\hbar}{m} \vec{k} \cdot \vec{p} + \frac{\hbar^2}{4m^2 c^2} (\vec{\nabla} V \times \vec{p}) \cdot \vec{\sigma}, \quad (A5.4)$$

and a $\vec{\nabla} V \times \vec{k}$ term has been neglected.

$$E_n' = E_n - \hbar^2 k^2 / (2m). \quad (A5.5)$$

The Pauli operation is $\vec{\sigma}$.

To solve for the required energies, the eigenvalues of an 8 x 8 matrix must be determined.

In Kane's notation we define:

$$P = -i \left(\frac{\hbar}{m} \right) \langle S | p_z | Z \rangle, \quad (A5.6)$$

and

$$\Delta \equiv \frac{3\hbar^2}{4m^2c^2} \langle X | \frac{\partial V}{\partial x} p_y - \frac{\partial V}{\partial y} p_x | Y \rangle, \quad (A5.7)$$

where the matrix elements involve s and p ($|X\rangle, |Y\rangle, |Z\rangle$) wave functions. If $\Delta \gg kP$, as seems to be appropriate for narrow band gap semiconductors, we get for the energy as measured from the bottom of the conduction band (neglecting a small term $\hbar^2 k^2 / 2m$):

$$E \equiv -E_g/2 + \sqrt{(E_g/2)^2 + \frac{2}{3} k^2 P^2}, \quad (A5.8)$$

where E_g is the energy gap between the conduction and the valence band.

Depending on the usage, various effective masses can be defined for spherical energy surfaces as above. We assume spherical energy surfaces and consistent with above (Chattopadhyay and Nag, (1974)):

$$E(1 + E/E_g) = \hbar^2 k^2 / 2m_0, \quad (A5.9)$$

where m_0 is the mass at the bottom of the conduction band

$$(m_0 = \frac{3\hbar^2 E_g}{4m P^2}).$$

Energy Effective Mass 1,

$$m_{E1} = \frac{\hbar^2 k^2}{2E}, \quad (A5.10)$$

Energy Effective Mass 2,

$$m_{E2} = \hbar^2 \left(\frac{d^2 E}{d k^2} \right)^{-1}. \quad (A5.11)$$

Momentum Effective Mass,

$$m_p = \hbar^2 k \left(\frac{dE}{dk} \right)^{-1}. \quad (A5.12)$$

($m_p \vec{v} = \hbar \vec{k}$ and \vec{v} and \vec{k} are parallel).
It is relatively easy to show

$$m_{E1}/m_0 = 1 + E/E_g, \quad (A5.13)$$

$$m_p/m_0 = 1 + 2E/E_g, \quad (A5.14)$$

$$m_{E2}/m_0 = (1 + 2E/E_g)^2 (1 - 2E/E_g)^{-1}, \quad (A5.15)$$

all three of these agree at the bottom of the conduction band ($E=0, k=0$).

Which one of these is appropriate depends on the usage.

The conventional effective mass as defined, for example, by Kittel (1986, p 194) is m_{E2} . The effective mass equation may be used as a starting point for discussing scattering in the Born approximation in solids. It would appear from a development of that equation (Madelung (1978), p. 79) that energy effective mass 1 could be the appropriate effective mass to use. For HgCdTe, m_p is typically about 10^{-2} of the mass of free electrons and has a strong dependence on carrier concentration and temperature.

By a standard development in the first Born approximation, the screening length comes out (see e.g. Patterson (1987)),

$$L_{m_{E1}}^{-2} = \frac{4e^2}{\pi \hbar^2} \int \left(-\frac{\partial f}{\partial E} \right) m_{E1} k dE. \quad (A5.16)$$

However, for this result to be applicable to non parabolic energy bands, the effective mass should be the momentum effective mass so that the density of states ($\rho(E)$) properly enters via

$$\rho(E) dE = \frac{1}{\pi^2} k^2 \frac{dk}{dE} dE \equiv \frac{m_p k}{\pi^2 \hbar^2} dE. \quad (A5.17)$$

Since $m_{E1} = \frac{1}{2} (m_p + m_0)$, (see above)

we find:

$$L_{m_{E1}}^{-2} = \frac{1}{2} (L_{m_p}^{-2} + L_{m_0}^{-2}) \quad (A5.18)$$

Then since

$$m_p > m_0 ,$$

$$L_{m_0}^{-2} \leq L_{m_p}^{-2} ,$$

we have

$$L_{m_{E1}}^{-2} \leq L_{m_p}^{-2} \quad (A5.19)$$

Hence a crude approach using the Born approximation could lead to a larger screening length, hence more scattering, hence less mobility.

Further Comment:

We also need to point out the usefulness of $\text{Hg}_{1-x}\text{Cd}_x$ as an infrared (IR) detector. Since

$$E = \hbar\omega = hc/\lambda ,$$

it is easy to show that

$$E_g \text{ (eV)} = 1.24/\lambda(\mu) . \quad (A5.20)$$

An important atmospheric window for IR is in the wavelength range 8-12 μ . At T=77K the energy gap is approximately (Dornhaus and Nimtz, 1983)

$$E_g = -.26 + 1.83x . \quad (A5.21)$$

We find that $.16 \leq x \leq .19$ will put us in the 8-12 μ window. There are other possibilities.

Appendix 6

Miscellany

a. Wigner Lattice

In an electron gas in which the kinetic energy is much less important than the potential energy, a localization or "crystallization" of the electrons can occur. It appears that this phenomena actually occurs at $x = .24$ in $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ at millikelvin temperature in a magnetic field (Rosenbaum et al. (1985)).

b. Layered Structures

One can make a superlattice consisting of alternating layers of CdTe and HgTe by use of molecular beam epitaxy. Such materials can be used as infrared detectors with properties that may be superior to $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ alloys (Berroir and Voos (1987)).

c. $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$

As this report reflects, $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ is the most important intrinsic semiconductor infrared detector material. $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$ has been considered as a possible competitor, because it may be more structurally stable. The use of $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$ is still quite new and much effort is being devoted to crystal growth techniques (Jozwikowski and Rogalski (1988)).